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Positron scattering from alkalis using a complex optical potential approach

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Abstract : The total cross sections for positron scattering from Li, Na, K, Rb and Cs are reported at positron energies in the range 10–1000 eV. A complex-optical-potential [$V_{opt}(r)$] approach is employed in which the real part (static plus polarization term) is calculated from Hartree-Fock target wave functions. The imaginary part of the optical potential *i.e.*, the absorption potential [$V^{+}_{abs}(r)$] which accounts for the loss of flux into inelastic channels, is derived semiempirically from the corresponding electron absorption potential [$V^{-}_{abs}(r)$] in the form $V^{+}_{abs}(r) = \frac{2}{(kr)^{2}} V^{-}_{abs}(r)$, where K is the wave number of the incident positron. The $V^{-}_{abs}(r)$ is taken from the work of Truhlar and coworkers. The $V_{opt}(r)$ is treated exactly in a partial wave analysis under the variable phase method. The effect of positronium formation channel, which opens at zero energy is neglected in the present work because in the considered energy range, its contribution to the total cross section is expected to be negligible. Our results of total cross section are in good accord with the available experimental results. We also compare our results with the other theoretical work.

Keywords : Positron scattering, alkali metals, optical potential.

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1. Introduction

The alkali metals can be represented as quasi one-electron systems because they are characterized by a loosely bound outer electron outside a closed shell. Due to the low ionization potentials of these elements, they exhibit large polarizabilities. Therefore, the incoming projectile (e^{-} or e^{+}) has significant effect in distorting the charge cloud of the target in the scattering calculations. Since the ionization potentials of alkali metals are less than the binding energy of the ground state of positronium, the positronium formation channel is open even at zero scattering energy. However, it has been established that for energies greater than 10 eV, the contribution of Ps formation to the total cross section is not very significant [1].

Historically, the alkali metals were the first elements in positron-atom scattering experiments. The main focus of these experiments was to compare the electron and positron total cross sections σ_t, at non-asymptotic energies [2–4]. Experimental total cross sections are available for positron impact on Na [3], K [2,3] and Rb [4]. On the theoretical side, Gien [5–7] has evaluated the σ_t for e^+ impact on Li, Na, K and Rb using the modified Glauber and the Second Born approximation in the energy range 10–1000 eV. Five state close-coupling calculations have been carried out by Ward *et al* [8] for e^+-Li, Na and K in the energy range 0.5–50 eV. McEachran *et al* [9] have calculated σ_t for e^+-Rb scattering, in a five state close-coupling with polarized frozen-core Hartree-Fock wavefunctions in the energy range 3.7 to 48.1 eV. McCarthy *et al* [10] have calculated σ_t for e^+ scattering on Na and K by employing coupled-channels-optical method with equivalent local polarization potential. In this approach, all channels are taken into account. They also included the effect of Ps formation and ionization. Mitroy and Ratnavelu [11] have generalised the close coupling theory of positron-hydrogen scattering to positron scattering from alkali atoms. They carried out calculations on e^+-Na scattering system in a model containing multiple sodium ($3s$, $3p$, $4s$, $3d$, $4p$) and Ps ($1s$, $2s$, $2p$) states in the energy range from threshold to 50 eV. Gianturco and Melissa [12] have used an optical potential approach to calculate cross sections for the Ps formation in Li, Na and K for positron energies upto 20 eV. Sarkar *et al* [13] have used an eigen state expansion method to study elastic and excitation processes for e^+-Na and e^+-Li scattering for energies upto 100 eV. Basu and Ghosh [14] have calculated elastic, excitation and Ps formation cross sections by using the three-state close-coupling approximation for e^+-Li scattering upto an energy of 100 eV.

In the present work, we have calculated σ_t for positron impact on all the alkali metals using an optical potential method. The energy range is 10–1000 eV. The effect of Ps formation is not taken into account as its contribution is expected to be small in the energy range considered in the present work.

2. Theory

In the optical model potential approach, the many body problem is reduced to an equivalent one body problem. The differential equation satisfying the scattering function $F(r)$ of the incident positron is

$$(\nabla^2 + k^2 - V_{opt}(r))\, F(r) = 0. \qquad (1)$$

The optical potential $V_{opt}(r)$ here is complex, nonlocal, nonspherically symmetric and energy dependent potential and k^2 is the energy of the incident positron. As the exact evaluation of $V_{opt}(r)$ is difficult, an approximate form is taken. In this work, we replace it by a spherically symmetric potential $V_{opt}(r)$ which takes care of closed and open channels. We express $V_{opt}(r)$ [15] as

$$V_{opt}(r) = V_{st}(r) + V_{pol}(r) + iV_{abs}(r). \qquad (2)$$

The imaginary part of $V_{opt}(r)$ accounts for absorption effects due to loss of flux in the open channels.

The static potential $V_{st}(r)$ is repulsive and is calculated at the Hartree-Fock level by employing the independent particle model [16] and is parametrized as

$$V_{st}(r) = \frac{\angle}{r}\Omega(r), \tag{3}$$

where the screening function $\Omega(r)$ is given by

$$\Omega(r) = \left[H(e^{r/d} - 1) + 1\right]^{-1}. \tag{4}$$

The parameters d and H for alkalis have been evaluated using Hartree-Fock eigen values [16].

We determine the polarization potential $V_{pol}(r)$ in the positron correlation polarization approximation (PCOP) which is based on the correlation energy of a single positron in a homogeneous electron gas [17]. Its short range part is different than the corresponding part of the e^- but asympotically both behave as $\frac{-\alpha_d}{2r^4}$ where α_d is the static dipole polarizability of the atom. Expressions for $V_{pol}(r)$ are available in different r regions [15]. The density for the atom is taken from independent atom model [16]

$$\rho(r) = \left((Z-1)/4\Pi r^2 d\right)\xi\left[He^{\xi}/(1+HT)^2\right]\left[-1+2He^{\xi}/(1+HT)\right], \tag{5}$$

where $T = e^{\xi} - 1$ and $\xi = r/d$.

We have used the absorption potential for e^- case [18–21] suitably modified for positron case. They are related as

$$V^{+}_{abs}(r) = \frac{\angle}{(kr)^{1/2}} V^{-}_{abs}(r). \tag{6}$$

In order to solve the radial Schrödinger equation, we transform it into a set of first order coupled differential equation and get the real and imaginary parts of the complex phase shift function under the variable phase approach. The elastic, inelastic and total cross sections are evaluated by standard formulas [15]. When the agreement between polarized Born phase shift and numerical phase shift is better than 0.1% at a particular value of partial wave say l_{max}, we switched over entirely to polarized Born phase shift for partial wave having value greater than l_{max}. At 1000 eV, 400 partial waves are used and convergence is tested by taking various step sizes.

3. Results and discussion

Figure 1 displays our σ_t values for e^+-Li scattering system for positron energies upto 1000 eV. There is no experimental data available. However, we have plotted the available theoretical results [5,8]. Gien [5] calculated σ_t by employing the modified Glauber approximation within the model potential approach for energies upto 1000 eV. There is a five-state close-coupling calculation [8] available in the energy range 0.5–50 eV. In this calculation, the states $2s$, $2p$, $3s$, $3p$ and $3d$ were included in the close-coupling expansion of the total wave-function of the scattering system. We have good agreement with the five-

state close-coupling [8] results. Beyond 20 eV, all the theoretical results merge with each other.

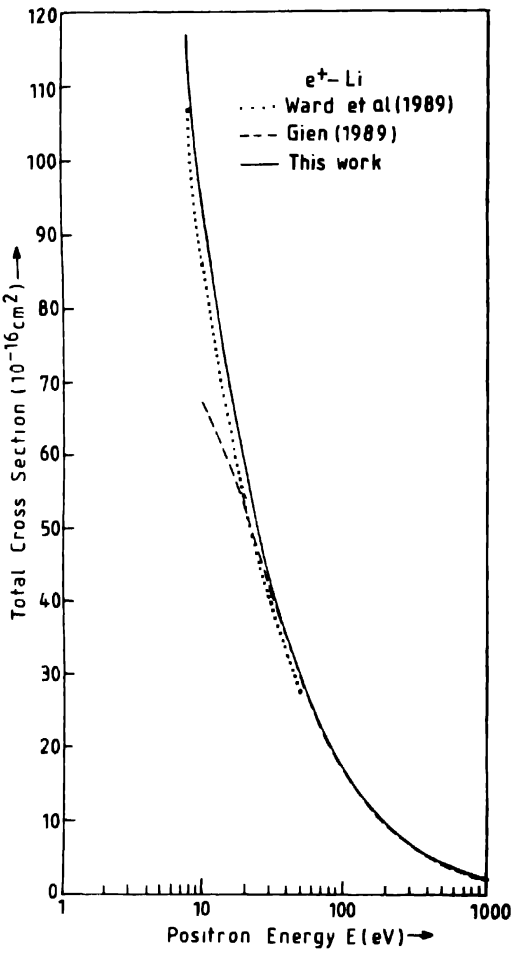

Figure 1. Total cross sections for positron impact on Li.

For e^+-Na, σ_t values are shown in Figure 2 along with the experimental points. Kwan *et al* [3] measured σ_t using beam transmission technique in the energy range 3–102 eV. There is good agreement between present theory and measurements at energies above 20 eV. At energies less than 10 eV, our curve lies above the measured points. Other theoretical calculations [5,8,10] are also shown in Figure 2. The agreement between our curve and the five-state (3*s*-3*p*-3*d*-4*s*-4*p*) close coupling [8] is fairly good even at low energies. Above 100 eV, modified-Glauber [5] results almost coincide with our theoretical

curve. The results of McCarthy *et al* [10] are in fair agreement with the experimental results. They used coupled-channel optical potential method with equivalent local polarization potential. Eight channels were coupled in this calculation. This method overestimates total cross sections at very low energies. Among all the theoretical calculations shown in Figure 2, our results lie closest to the experimental results for

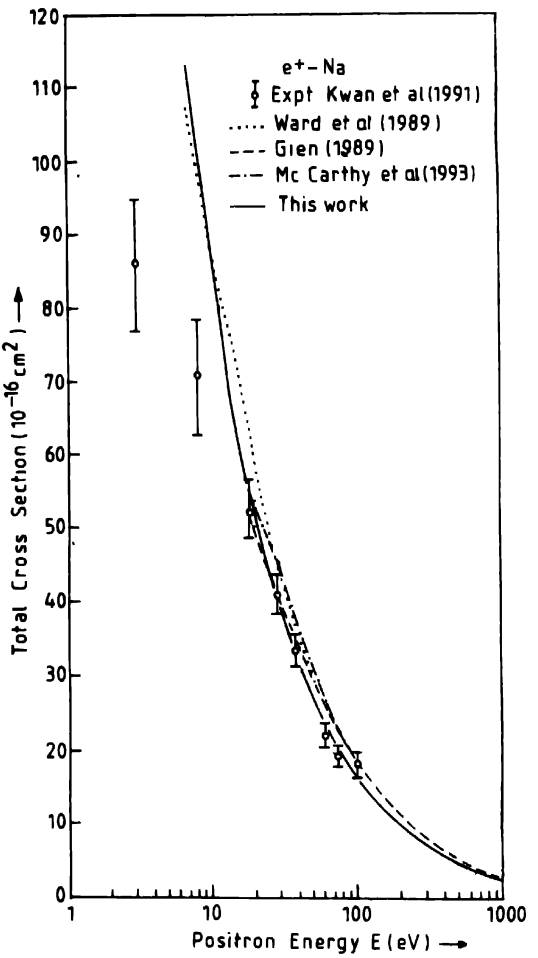

Figure 2. Total cross sections for positron impact on Na.

energies greater than 20 eV. No theory is capable of reproducing experimental results at energies less than 20 eV. We must point out that in the experimental measurements at low energies there is a serious problem for accounting the flux of positrons which are elastically scattered through the small angles in the forward direction. The close-coupling method is

particularly appropriate for e^+-alkali scattering because the lowest P state alone accounts for 97% of the static dipole polarizability which means that the effect of continuum is negligible and the close-coupling method for e^+-alkali system is fairly rapid with respect to the number of bound states included in the close-coupling expansion. It is indeed very satisfying to note that our optical potential model is capable of giving σ_t values which are in good accord with close-coupling results in the low as well as in the intermediate energy region.

The σ_t values for e^+-K system are displayed in Figure 3 where our values along with other theoretical calculations [5, 6, 8, 10, 11] are compared with the observed results [2, 3].

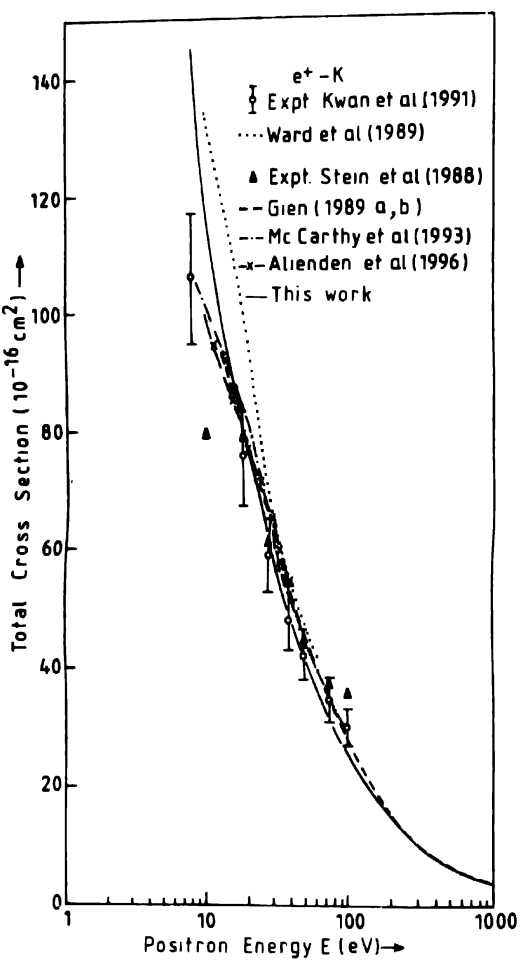

Figure 3. Total cross sections for positron impact on K.

We have good agreement with the experimental results for energies greater than 20 eV. We also have fair agreement with the five-state calculation [8]. Beyond 100 eV, the modified Glauber results [5] merge with our results. Recently, a coupled state calculation [22] involving $4s$, $4p$, $5s$, $5p$, $3d$ states of potassium and $1s$, $2s$, $2p$, $3s$, $3p$, $3d$ states of Ps formation has been repored in the energy range 0.5–60 eV. This calculation yields σ_t values which are slightly larger than our values for energies greater than 20 eV. Since Ps formation cross sections are not significant beyond 30 eV, it is fair to conclude that our model which neglects Ps formation channel, yields reliable results for energies greater than 30 eV.

In Figure 4, we have shown theoretical σ_t values for e^+ impact on Rb along with the beam transmission results [4]. Once again, our model predicts σ_t values which are in good

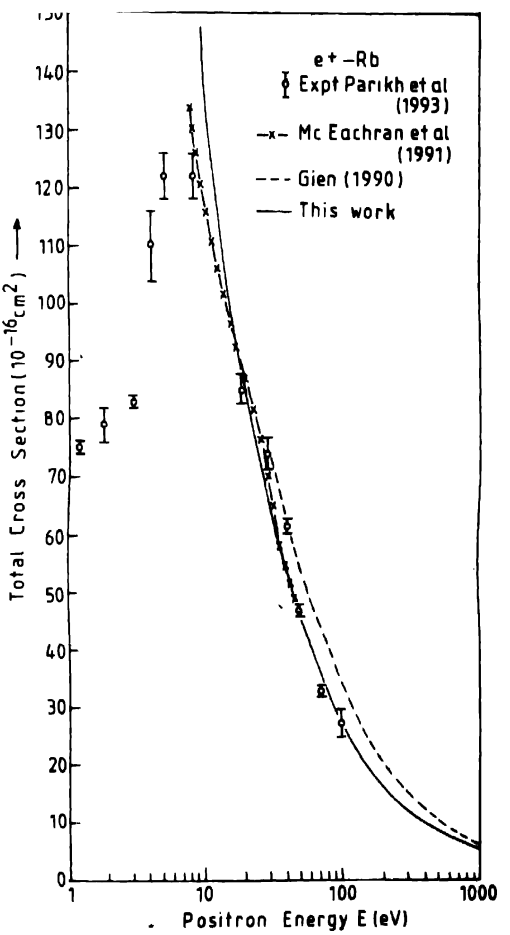

Figure 4. Total cross sections for positron impact on Rb.

accord with the experimental values for energies greater than 20 eV. The modified Glauber [7] results lie somewhat higher than our results. We have also shown the effective σ_t values of a five-state close-coupling calculation [9] using polarized frozen-core Hartree-Fock wavefunctions. The effective total cross section is the total integrated cross section minus the cross section for undiscriminated elastically scattered positrons. Their results are in good agreement with the experimental results but at lower energies, they increase with decreasing energy. The experimental peak around 7 eV cannot be reproduced by any theoretical model. This remains a challenge for more theoretical work.

Our σ_t values for e^+-Cs are shown in Figure 5. The cross sections decrease monotonically with increasing energy. There are no other theoretical and experimental

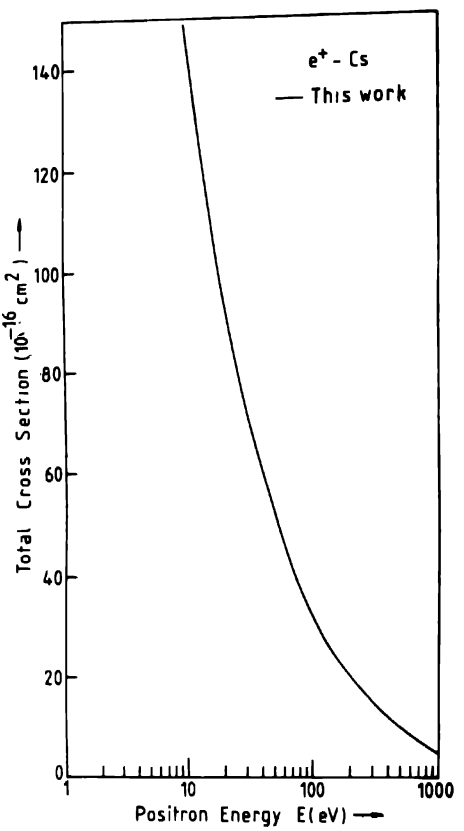

Figure 5. Total cross sections for positron impact on Cs.

results available to compare with our results. Since our work on other alkali atoms have shown that our model yields σ_t values which are in good agreement with experimental

results, we believe that our σ_t values for e^+-Cs should be quite reliable. For the sake of convenience of other workers, we have tabulated our results in Table 1.

Table 1. Total cross sections (in 10^{-16} cm^2) for e^+ impact on alkali metals.

Energy (eV)	Li	Na	K	Rb	Cs
10	97.37	87.20	122.20	137.16	148.05
30	43.36	38.59	58.61	65.36	74.02
50	28.80	27.15	40.05	46.033	52.67
70	23.08	21.07	32.71	36.95	42.21
100	17.31	16.76	25.16	28.74	32.84
200	9.68	10.08	14.71	17.19	19.66
400	5.44	6.06	8.86	10.09	12.03
600	3.79	4.05	6.13	7.65	8.01
800	2.75	3.21	4.69	6.25	6.15
1000	2.34	2.41	3.79	5.28	4.82

4. Conclusion

We have calculated σ_t values for e^+ scattering on alkali metals using an optical potential model in which the loss of flux from the elastic channel to inelastic channels is accounted for by an absorption potential which is modified approximately for the positron case. We have also employed a polarization potential which is positron specific. Our σ_t values are in good agreement with the observed results for all the alkalis for positron impact energies greater than 20 eV. Since our results also match closely with the five-state close-coupling results, it is fair to conclude that our optical potential model has all the essential physical ingredients built into it. Further theoretical work should be undertaken to produce better results at energies below 10 eV so that more light is shed specifically on the peak around 7 eV for e^+-Rb system. A similiar peak may also be present for e^+-Cs system around 5 eV.

Acknowledgments

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